FINGERPRINTS OF INTRAMOLECULAR HYDROGEN BONDS: SYNCHROTRON-BASED FAR IR STUDY OF THE CIS AND TRANS CONFORMERS OF 2-FLUOROPHENOL

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Rotationally-resolved vibrational spectra of two planar conformers of 2-fluorophenol have been collected from 100-1000 cm^{-1} using the Bruker IFS125HR FTIR spectrometer at the Canadian Light Source with a resolution of 0.000959 cm^{-1}. The cis conformer is lower in energy by 2.9 kcal/mol (MP2/aug-cc-pvDZ) and is thought to be stabilized by an intramolecular hydrogen bond between the hydroxyl group and neighbouring fluorine atom on the ring. The OH out-of-plane torsion bands below 400 cm^{-1} provide the best fingerprint to distinguish between the two conformers in the gas phase spectrum as the *c*-type band origin of the cis conformer is blue-shifted by 36 cm^{-1} from that of the trans conformer as result of the intramolecular interaction. In this talk, we will discuss the progress of the analysis of this complex far infrared spectrum of 2-fluorophenol.